

BOUNDARY CONDITIONS FOR THE PALEOENVIRONMENT: CHEMICAL AND
PHYSICAL PROCESSES IN DENSE INTERSTELLAR CLOUDS

SUMMARY OF RESEARCH (FINAL REPORT)

NASA GRANT NAG5-3653

OCTOBER 15, 1996- OCTOBER 14, 1999
(including no-cost extension)

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Summary:

The basic theme of this program was the study of molecular complexity and evolution for the biogenic elements and compounds in interstellar clouds and in primitive solar system objects. Research included the detection and study of new interstellar and cometary molecules and investigation of reaction pathways for astrochemistry from a comparison of theory and observed molecular abundances. The latter includes studies of cold, dark clouds in which ion-molecule chemistry should predominate, searches for the effects of interchange of material between the gas and solid phases in interstellar clouds, unbiased spectral surveys of particular sources, and systematic investigation of the interlinked chemistry and physics of dense interstellar clouds. In addition, the study of comets has allowed a comparison between the chemistry of such minimally thermally processed objects and that of interstellar clouds, shedding light on the evolution of the biogenic elements during the process of solar system formation.

One PhD dissertation on this research was completed by a graduate student at the University of Massachusetts. An additional 4 graduate students at the University of Massachusetts and 5 graduate students from other institutions participated in research supported by this grant, with 6 of these thus far receiving PhD degrees from the University of Massachusetts or their home institutions. Four postdoctoral research

associates at the University of Massachusetts also participated in research supported by this grant, receiving valuable training.

Research Results:

New interstellar and cometary molecules:

The identification of new interstellar and cometary molecules increases our knowledge of the chemical complexity of these objects and hence guides models of their origin and evolution. We have participated in the recent discovery one new interstellar molecule, ethylene oxide ($c\text{-C}_2\text{H}_4\text{O}$), and one new cometary molecule, hydrogen isocyanide (HNC).

Graduate student J. Dickens, Principal Investigator Irvine, and colleagues in Japan and Sweden identified only the third known cyclic molecule in interstellar clouds, ethylene oxide, in the Galactic center cloud SgrB2. Ethylene oxide is a higher energy isomer of the known interstellar molecule acetaldehyde (CH_3CHO). A subsequent survey for ethylene oxide and acetaldehyde in molecular clouds led to their joint detection in 5 "hot cores", confined regions in the immediate vicinity of very young, massive stars. The combined abundances of these isomers is larger than the predictions of recent gas phase chemical models. This suggests that the production of these organic molecules involves grain-mediated processes, consistent with previous suggestions for species such as ethanol.

The high abundance of hydrogen isocyanide (HNC) in cold interstellar clouds, relative to its more stable isomer hydrogen cyanide (HCN), has long been regarded as a hallmark of ion-molecule interstellar chemistry. Thinking, therefore, that the presence of HNC in comets might signal the preservation of interstellar molecular material, which would in turn provide important constraints on cometary formation and evolution, we searched for and detected this molecule in Comet Hyakutake (C/1996 B2). Alternative, non-interstellar origins for the HNC were, however, conceivable. A discriminant among possible origins for HNC would be the dependence of the HNC/HCN ratio on heliocentric distance: if both HCN and HNC were present in the nuclear ices, one would expect that their abundance ratio would be independent of heliocentric distance; on the other hand, if HNC were produced in the coma by processes ultimately dependent on the solar radiation field, the HNC/HCN ratio should increase as a comet approaches the Sun. We found for comet Hale-Bopp that the

HNC/HCN ratio varied with heliocentric distance in a way that can be matched with a gas phase chemical model of the coma, but not if the HNC is a nuclear constituent. Thus, HNC is the first neutral molecule whose origin in active comets can be ascribed in large part to chemical reactions in the coma.

Chemical surveys:

Survey projects can provide crucial fundamental data for understanding chemical processes in astronomical contexts. Two types of surveys have been undertaken: unbiased spectral surveys of specific astronomical sources; and high resolution mapping of molecular clouds in many molecular transitions.

A particularly interesting region to survey is the Galactic center cloud SgrB2, probably the most massive molecular cloud in the Galaxy. In order to probe the chemical gradients in this region and relate them to variations in physical properties, three positions have been studied in the 1mm wavelength band in a collaboration with astronomers from Sweden and Japan. Two positions appear to be the sites of ongoing formation of massive stars, while the third appears more similar to a quiescent dark cloud. The two star formation sites differ between themselves, however, with sulfur-containing molecules being prominent in the spectrum in one case, and complex organic molecules in the other location. A large number of previously unreported emission lines assignable to known interstellar molecular species have been detected; in addition, a number of unidentified lines are apparent.

A different type of survey has been undertaken toward two dark clouds of the type where solar-mass stars form. In a collaboration involving several astronomers at the University of Massachusetts, Taurus Molecular Cloud One (TMC-1) and Lynds 134 North (L134N) have been mapped in 33 molecular transitions of 21 molecular species and isotopomers. This integrated approach was only possible with the aid of the unique capabilities of the focal plane array receiver on the University of Massachusetts' 14m telescope. The goal was to investigate the interlinked chemistry and physics over these extended regions. Previous research had suggested that these two clouds had similar physical properties (kinetic temperature and density) but differing compositions. For TMC-1 clear abundance gradients are present, which can be well

matched by current theories for a small density gradient. For the other cloud, L134N, the observations are complete and analysis is underway.

Probing chemical processes:

Molecules with identical hydrogen atoms, such as formaldehyde (H_2CO), can exist in either the ortho or the para symmetry species depending on whether the spins of the hydrogen nuclei are parallel (ortho) or anti-parallel (para). The relative abundance of the two species defines the spin temperature, which contains information on the formation process of the molecule. Formaldehyde is a good probe of such processes in cold, dark interstellar clouds, since the energy difference between the lowest ortho and the lowest para state is only 15 K. Dickens and Irvine measured the formaldehyde ortho/para ratio in several dark clouds and found a consistent difference in the spin temperature between those clouds which contained embedded young stellar objects and those which lacked such evidence for low-mass star formation. They attributed the difference to the release of formaldehyde from icy grain mantles in the regions heated by embedded stars, a conclusion supported by the enhanced H_2CO abundance in such clouds.

Chemistry of comets:

Comets may well have provided a substantial portion of the volatile budgets of the terrestrial planets, perhaps including organic matter that might have played a role in the origin of life on Earth. The apparitions in 1996 and 1997 of comets Hyakutake and Hale-Bopp provided the opportunity to utilize modern instrumentation to study two of the brightest comets of the century.

In addition to the study of the HNC/HCN ratio in comets mentioned above, the importance of coma chemistry was emphasized by the maps of molecular emission for comets Hyakutake and Hale-Bopp obtained with the unique 3mm-wavelength focal plane array at the University of Massachusetts' radio observatory. These observations provided the first cometary images of molecular emission from the HCO^+ ion and from HCN and CS . For HCO^+ the minimum in brightness towards the nucleus and the large emission region clearly illustrated the chemical production and destruction processes occurring in the coma gas. The NRAO 140-ft. radio telescope in Green Bank was used to observe the OH radical, in order to

monitor the water production in these comets and to study the physical processes associated with OH maser emission.

Postdoc M. Senay participated in observations showing that the DCN/HCN ratio in comet Hale-Bopp is some two orders of magnitude larger than the cosmic D/H ratio, supporting an interstellar origin for some cometary ices and constraining the temperature in the region of cometary formation.

Reviews:

Irvine presented an invited review on "Extraterrestrial Organic Matter" at the Fifth Chemical Congress of North America in Cancun, Mexico, in 1997. He reviewed "Chemistry in Cometary Comae" at Faraday Discussion 109 of the Royal Society of Chemistry in Nottingham, UK, in April, 1998, and he (and co-authors) presented the invited paper "Comets: A Link between Interstellar and Nebular Chemistry" at the conference Protostars and Planets IV at Santa Cruz, CA, in July, 1998. Irvine delivered a talk on "Molecules in Interstellar Molecular Clouds" in September, 1998, at a Workshop on the Origin and Composition of Cometary Material, organized by the International Space Institute in Bern, Switzerland. He presented a review of recent research on volatiles in comets entitled "Molecules in Comets: An ISM-Solar System Connection?" at International Astronomical Union Symposium 197 on Astrochemistry in Sogwipo, South Korea, in August, 1999. All of these reviews except the first-mentioned have been refereed and are published or in press.

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